Space-time dispersion of graphene conductivity

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We present an analytic calculation of the conductivity of pure graphene as a function of frequency ω , wave-vector k, and temperature for the range where the energies related to all these parameters are small in comparison with the band parameter $\gamma=3$ eV. The simple asymptotic expressions are given in various limiting cases. For instance, the conductivity for $kv_0 \ll T \ll \omega$ is equal to $\sigma(\omega,k)=e^2/4\hbar$ and independent of the band structure parameters γ and v_0 . Our results are also used to explain the known dependence of the graphite conductivity on temperature and pressure.

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INTRODUCTION

Recently the properties of graphene attracted special attention (see, for instance [1] and references therein). The matter of fact the wide variety of carbon materials such as graphite, graphene tubules, and fullerenes consists of graphene (i.e., a single layer of graphite) sheets shaped in different manner.

Two-dimensional graphene has a very simple band structure, which can be obtained with help of the symmetry consideration or in tight-binding approximation [2]. It was shown in Refs. [3, 4] that the energy bands of graphene are degenerated at the corners of the 2D Brillouin zone $K=(0,4\pi/3\sqrt{3}a)$, where a=1.44 Å is the interatomic distance (see Fig. 1). This is the Dirac-type spectrum but it is massless and two-dimensional. It was demonstrated that due to the symmetry arguments such gapless spectrum with the conic point in the 3D case turns out stable with respect to the Coulomb interaction [5]. One can proof that this stability remains also for the 2D graphene spectrum with the conic point. Such

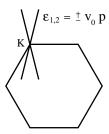


FIG. 1: The Brillouin zone of graphene and the electron spectrum in the vicinity of the K points

simple band structure can be used in analytic calculations of various thermodynamic and transport properties of graphene. An example of such calculations was presented in Ref. [6] where the imaginary part of the dielectric function $\text{Im}\varepsilon(\omega)$ of graphite has been calculated. The gapless band structure of graphene also results in the unusual behavior of conductivity. Despite the enor-

mous number of paper devoted to carbon materials, the analytical expression of graphene conductivity was not yet derived to our best knowledge.

The standard diagrammatic approach to calculation of transport properties of impure metals is restricted by the fundamental requirement that the mean free path of carriers $\ell = v_0 \tau$ must be much larger than the electron wavelength $\lambda = h/p_F$, i.e. $\ell p_F \gg 1$. This condition cannot be evidently satisfied in the case of graphene when the Fermi surface degenerates to the points. We avoid this difficulty addressing the problem when the graphene sample is clean enough but temperature is finite $(T\tau \gg 1)$. In this case the temperature appears instead of Fermi energy and electrons obey Boltzmann statistics.

In the present paper, we calculate analytically the frequency and wave-vector dependence of the graphene conductivity $\sigma_{ij}(\omega, k)$ at finite temperature T for the relatively low frequencies $\omega \ll 3$ eV, when only the nearest π bands can be taken into consideration.

HAMILTONIAN AND CURRENT

Let us remind briefly the properties of the graphene electron spectrum. The tight-binding approximation allows to write down the following effective Hamiltonian 2×2 matrix

$$H(\mathbf{p}) = \begin{pmatrix} 0 & h(\mathbf{p}) \\ h^*(\mathbf{p}) & 0 \end{pmatrix}, \tag{1}$$

where $h(\mathbf{p}) = \gamma \left\{ e^{ip_x a} + 2e^{-ip_x a/2} \cos\left(p_y a\sqrt{3}/2\right) \right\}$ and $\gamma = \langle \psi(a,0)|H_0|\psi(0,0) \rangle$ is the $pp\pi$ transfer integral, which is of the order of 3 eV. The dispersion law of graphene, $\varepsilon_{1,2}(\mathbf{p})$ can be obtained by means of its diagonalization:

$$\varepsilon_{1,2}(\mathbf{p}) = \pm \gamma \left\{ 1 + 4\cos(3p_x a/2)\cos(p_y a\sqrt{3}/2) + 4\cos^2(p_y a\sqrt{3}/2) \right\}^{1/2}.$$
(2)

In the vicinity of the K point, the matrix elements of the effective Hamiltonian can be expanded as

$$h(\mathbf{p}) = v_0(ip_x + p_y),$$

where $v_0 = 3\gamma a/2$. This results in the linear dispersion relation $\varepsilon_{1,2}(\mathbf{p}) = \pm v_0 p$. Calculating the conductivity, we can use this expansion for $\omega \ll \gamma \approx 3$ eV. Let us pass to the calculation of the electric current, following the paper by Abrikosov [7], where the dielectric function of Bi-type metals was considered. We assume that the external field is described by the vector potential A_j . The current operator has the form

$$j_{i}(x) = e\tilde{\psi}^{+}(x')v_{x'x}^{i}\tilde{\psi}(x) - \frac{e^{2}}{c}\tilde{\psi}^{+}(x')(m^{-1})_{x'x}^{ij}\tilde{\psi}(x)A_{j}$$
(3)

where $x' \to x$, $v^i_{x'x}$ and $(m^{-1})^{ij}_{x'x}$ are the velocity and mass operators correspondingly, the tilde in the notation $\tilde{\psi}$ means that the operator is taken in the interaction representation with

$$V = -\frac{e}{c} \int \psi^{+}(x') v_{x'x}^{i} \psi(x) A_{i}(x) d^{4}x.$$
 (4)

We will calculate the current in the linear approximation in $A_i(x)$. Therefore, the second term in Eq. (3) can be taken in zeroth approximation with respect to the interaction (4). Expanding the first term in Eq. (3) to the first order in $A_i(x)$, we get the retarded correlator of four $\tilde{\psi}$ operators which has to be averaged over the Gibbs ensemble. At finite temperatures, the Fourier component (with respect to the spatial coordinates and imaginary time) of this correlator

$$\mathcal{P}(\omega_l, \mathbf{k}) = \sum_{\omega_n} \int \frac{d^2 \mathbf{p}}{(2\pi)^2} Tr \left\{ v^i \mathcal{G}(p_+) v^j \mathcal{G}(p_-) \right\}$$
 (5)

is expressed in terms of the temperature Green's functions:

$$\mathcal{G}(p) = \left[i\omega_n - H(\mathbf{p})\right]^{-1}$$

In Eq. (5) the notations p_{\pm} are used, the summation is carried out over the fermionic frequencies $\omega_n = 2\pi T (n+1/2)$, while the trace operation is performed over the band index of the Hamiltonian $H(\mathbf{p})$. The latter can be easily carried out in the representation where the Hamiltonian has diagonal form:

$$Tr\left\{v^{i}\mathcal{G}v^{j}\mathcal{G}\right\} = v_{11}^{i}\mathcal{G}_{11}v_{11}^{j}\mathcal{G}_{11} + v_{22}^{i}\mathcal{G}_{22}v_{22}^{j}\mathcal{G}_{22}$$

$$+v_{12}^{i}\mathcal{G}_{22}v_{21}^{j}\mathcal{G}_{11}+v_{21}^{i}\mathcal{G}_{11}v_{12}^{j}\mathcal{G}_{22}.$$

Then one can perform the summation over ω_n in standard way. For instance, for the cross product of the Green

functions one finds

$$T \sum_{\omega_n} \mathcal{G}_{11}(p_+) \mathcal{G}_{22}(p_-) = \frac{T}{i\omega_l - \varepsilon_2(\mathbf{p}_+) + \varepsilon_1(\mathbf{p}_-)}$$
(6)
$$\times \sum_{\omega_n} \left[\frac{1}{i\omega_- - \varepsilon_1(\mathbf{p}_-)} - \frac{1}{i\omega_+ - \varepsilon_2(\mathbf{p}_+)} \right]$$

$$= \frac{f_0[\varepsilon_1(\mathbf{p}_-)] - f_0[\varepsilon_2(\mathbf{p}_+)]}{i\omega_l - \varepsilon_2(\mathbf{p}_+) + \varepsilon_1(\mathbf{p}_-)},$$

where we have taken into account that the photon frequencies $\omega_l = 2\pi l T$ are "even" in the Matsubara technique; f_0 is the Fermi distribution function. Analytical continuation of the expressions similar to Eq. (7) into the upper half plane of the complex frequency can be performed by simple substitution $i\omega_l \to \omega + i\delta$ with $\delta \to 0$.

Let us notice that the current has to vanish when the vector potential does not vary in time. Since the second term in Eq. (3) is time independent, one can omit it, subtracting from the first term its value at $\omega = 0$. In result

$$\sigma_{ij}(\omega, k) = \frac{ie^2}{\pi^2} \times$$

$$\left\{ \sum_{a=1,2} \int \frac{d^2 p v^i v^j \{ f_0[\varepsilon_a(\mathbf{p}_-)] - f_0[\varepsilon_a(\mathbf{p}_+)] \}}{[\varepsilon_a(\mathbf{p}_+) - \varepsilon_a(\mathbf{p}_-)][\omega - \varepsilon_a(\mathbf{p}_+) + \varepsilon_a(\mathbf{p}_-)]} \right.$$

$$\left. + 2\omega \int \frac{d^2 p v_{12}^i v_{21}^j \{ f_0[\varepsilon_1(\mathbf{p}_-)] - f_0[\varepsilon_2(\mathbf{p}_+)] \}}{[\varepsilon_2(\mathbf{p}_+) - \varepsilon_1(\mathbf{p}_-)] \{ \omega^2 - [\varepsilon_2(\mathbf{p}_+) - \varepsilon_1(\mathbf{p}_-)]^2 \}} \right\}.$$

This expression acquired the factor 4 due to summation over spin and over six points of the K type (two per each Brillouin zone).

Hitherto we did not use any peculiarities of the graphene spectrum besides the number of bands. Thus Eq. (7) has a general character. For graphene, the matrix of the velocity near the point K in the band representation is determined by the Hamiltonian (1):

$$\mathbf{v} = v_0 \begin{pmatrix} 0 & -\mathbf{e}_y + i\mathbf{e}_x \\ -\mathbf{e}_y - i\mathbf{e}_x & 0 \end{pmatrix}, \tag{8}$$

where \mathbf{e}_i are unit vectors along the coordinate axis directions. The unitary transformation which transforms the Hamiltonian from the band representation to the diagonal one has the form

$$U = \frac{1}{\sqrt{2}p} \left(\begin{array}{cc} p_y - ip_x & p_y - ip_x \\ -p & p \end{array} \right).$$

Its application to the velocity matrix gives:

$$U^{-1}\mathbf{v}U = \frac{v_0}{p} \begin{pmatrix} \mathbf{e}_x p_x + \mathbf{e}_y p_y & i(\mathbf{e}_x p_y - \mathbf{e}_y p_x) \\ -i(\mathbf{e}_x p_y - \mathbf{e}_y p_x) & -\mathbf{e}_x p_x - \mathbf{e}_y p_y \end{pmatrix}.$$

The first term in Eq. (7) corresponds to the intra-band electron-photon scattering processes. In the limit of the

high carriers concentration $kv_0 \ll (T, E_F)$, it leads to the usual Drude expression

$$\sigma_{xx}^{intra}(\omega, 0) = \frac{e^2}{(i\omega - \tau^{-1})} \sum_{a=1,2} \int \frac{d^2p}{2\pi^2} v_{ax}^2 \frac{df_0\left[\varepsilon_a(\mathbf{p})\right]}{d\varepsilon},$$
(9)

with $1/\tau \to 0$ (τ is the transport scattering time). The second term in Eq. (7) owes its origin to the inter-band electron transitions. The real part of this contribution (let us recall, that $i\omega_l \to \omega + i\delta$) at $k \to 0$ is reduced to the well-known expression for the absorbed energy due to the direct inter-band transitions.

ASYMPTOTIC BEHAVIOR OF CONDUCTIVITY

Let us pass to the discussion of the the pure graphene conductivity in absence of gate voltage, when the chemical potential is equal to zero. The integral (7) can be performed analytically for various limiting cases.

Small spatial dispersion $kv_0 \ll \omega, T$

Putting k=0 and integrating over angle, one can find that the off-diagonal elements of conductivity vanish, while the diagonal ones are equal to:

$$\sigma_{xx}(\omega,0) = \sigma_{yy}(\omega,0) = -\frac{ie^2\omega}{\pi} \times \left[\frac{2}{\omega^2} \int_0^\infty \varepsilon d\varepsilon \left(\frac{df_0(\varepsilon)}{d\varepsilon}\right) - \int_0^\infty d\varepsilon \, \frac{f_0(-\varepsilon) - f_0(\varepsilon)}{\omega^2 - 4\varepsilon^2}\right].$$

The first (intra-band) contribution:

$$\sigma_{xx}^{intra}(\omega, k) = 2 \ln 2 \frac{ie^2 T}{\pi \hbar \omega}, \quad k v_0 << \omega, T$$
 (10)

(we write explicitly the Planck constant in the final expressions). This result was obtained in Ref. [3] using the Drude expression, Eq. (9).

The inter-band term in Eq. (10) has the form:

$$\sigma_{xx}^{inter}(\omega, 0) = \frac{e^2}{4} \tanh \frac{\omega}{4T}$$

$$+ \frac{ie^2 \omega}{\pi} P \int_0^\infty \frac{d\varepsilon}{\omega^2 - 4\varepsilon^2} \tanh \frac{\varepsilon}{2T},$$
(11)

where P denotes the operation of taking the principal value of an integral. This integral can be presented in more convenient form

$$I_P = P \int_0^\infty \frac{d\varepsilon}{\omega^2 - 4\varepsilon^2} \left[\tanh \frac{\varepsilon}{2T} - 1 \right]$$
$$= -2P \int_0^\infty \frac{d\varepsilon}{(\omega^2 - 4\varepsilon^2)(\exp(\varepsilon/T) + 1)}.$$

In the limit of low temperatures $T<<\omega$, the energies $\varepsilon\sim T<<\omega$ are essential and we can take Taylor of the integrand over T/ω :

$$I_P = -\frac{2T}{\omega^2} [\ln 2 + 6\zeta(3)(T/\omega)^2],$$
 (12)

where $\zeta(3) = 1.20$. One can see that the term with $\ln 2$ exactly cancels the intra-band contribution (10).

In the limit of high temperatures $T >> \omega$, the leading contribution to the integral (11) originates from the region $\omega < \varepsilon < T$. One can obtain with the logarithmic accuracy:

$$I_P = -\frac{1}{8T} \int_{0}^{T} \frac{d\varepsilon}{\varepsilon} = -\frac{1}{8T} \ln \frac{T}{\omega}.$$
 (13)

Collecting the Eqs. (11),(12), and (13), one can write:

$$\sigma_{xx}^{inter}(\omega, k) = \frac{e^2}{4\hbar} \tanh \frac{\omega}{4T} - \frac{2ie^2}{\pi\hbar} \times (14)$$

$$\begin{cases} (T/\omega)[\ln 2 + 6\zeta(3)(T/\omega)^2], & kv_0 << T << \omega, \\ (\omega/16T)\ln(T/\omega), & kv_0 << \omega << T. \end{cases}$$

Large spatial dispersion $\omega \ll kv_0, T$

Now let us consider the limit of large dispersion $kv_0 >> \omega$. We choose the direction of **k** along the x-axis. In the intra-band term of Eq. (7), one can expand

$$\varepsilon_{2,1}(\mathbf{p}_{\pm}) = \sqrt{\varepsilon^2(p) + (v_0 k/2)^2 \pm pkv_0^2 \cos \phi} \approx (15)$$
$$\varepsilon_0(p) \pm pkv_0^2 \cos \phi/2\varepsilon_0,$$

where $\varepsilon_0(p) = \sqrt{\varepsilon^2(p) + (v_0 k/2)^2}$, $\varepsilon(p) = v_0 p$, and ϕ is the angle between **k** and **p**.

Now we evaluate the integral in the Eq. (7) for $\sigma_{xx}^{intra}(\omega, k)$. First of all, let us note that changing of the variable of integration $\mathbf{p} \to -\mathbf{p}$ results in

$$= \frac{[\omega - \varepsilon_a(\mathbf{p}_+) + \varepsilon_a(\mathbf{p}_-)]^{-1} + [\omega + \varepsilon_a(\mathbf{p}_+) - \varepsilon_a(\mathbf{p}_-)]^{-1}}{2\omega}$$
$$= \frac{2\omega}{\omega^2 - [\varepsilon_a(\mathbf{p}_+) - \varepsilon_a(\mathbf{p}_-)]^2}.$$

Using the expansion (15) one can see that in the significant domain of integration, determined from the condition $\omega \ll pkv_0^2/\varepsilon_0(p)$, the integrand of intra-band part σ_{xx}^{intra} in Eq. (7), can be presented as follows

$$v_x^2 \frac{df_0(\varepsilon_0)}{d\varepsilon_0} \frac{\omega \varepsilon_0^2}{(pkv_0^2 \cos \phi)^2},$$

where $v_x=v_0\cos\phi$. Thus, $\cos\phi$ disappears in the integrand. But for the intra-band contribution in the transversal σ_{yy}^{intra} component of conductivity, we have $v_y=v_0\sin\phi$, and therefore, the longitudinal and

transversal components (respect with the ${\bf k}$ - direction) are different:

$$\sigma_{xx}^{intra}(\omega, k) = \frac{-ie^2\omega}{\pi\hbar T} \times$$

$$\begin{cases} (2T/kv_0)^2 \ln 2, & \omega < kv_0 < T, \\ \ln(2\sqrt{kv_0T}/\omega) \exp(-kv_0/2T), & \omega < T < kv_0, \end{cases}$$

$$\begin{split} \sigma_{yy}^{intra}(\omega,k) &= \frac{e^2}{\pi\hbar} \times \\ \left\{ \begin{array}{ll} (4T/kv_0) \ln 2, & \omega < kv_0 < T, \\ \sqrt{\pi kv_0/T} \exp{(-kv_0/2T)}, & \omega < T < kv_0. \end{array} \right. \end{split}$$

What concerns the inter-band contribution, here we can put $\varepsilon_{2,1} = \pm \varepsilon_0(p)$. Taking into account that $v_{12}^x = iv_0 \sin \phi$ and integrating over ϕ , one can obtain

$$\sigma_{xx}^{inter}(\omega, k) = \frac{-ie^2\omega}{4\pi} \int_{kv_0/2}^{\infty} \frac{d\varepsilon_0}{\varepsilon_0^2} \tanh \frac{\varepsilon_0}{2T}.$$

Evaluating this integral, we obtain for the inter-band contribution

$$\begin{split} \sigma_{xx}^{inter}(\omega,k) \; = \; \sigma_{yy}^{inter}(\omega,k) = -\frac{ie^2\omega}{2\pi\hbar} \times \\ \left\{ \begin{array}{ll} (1/4T)\ln{(4T/kv_0)}, & \omega < kv_0 < T, \\ 1/kv_0, & \omega < T < kv_0. \end{array} \right. \end{split}$$

CONCLUSIONS

The expression Eq. (14) allows us to estimate the conductivity of pure graphene, $\tau^{-1}=0$. In this case, the first term plays the leading role (for small k and at low temperatures, when $\tanh \omega/T=1$:

$$\sigma(\omega, k) = \frac{e^2}{4\hbar}, \quad kv_0 \ll T \ll \omega.$$
 (16)

Let us underline that this conductivity results from the electron transitions between two intersecting bands at the K points of the Brillouin zone. Remarkable fact is that its value turns out to be universal, independent of any parameter of graphene, like γ_0 or v_0 .

Very recently the electric field effect in graphene was investigated experimentally [1]. Indeed, the universal conductivity behavior for the samples with different carrier concentrations was found. In spite of fact that the experiment was performed in conditions $\omega \ll T$, different from Eq. (16), the minimal value of measured conductivity $\sigma^{(\min)} = 2e^2/\pi\hbar$ was found close to our prediction.

At high temperatures, when the condition $kv_0 \ll \omega \ll T$ is fulfilled, the conductivity Eq. (10) becomes imaginary:

$$\sigma(\omega, k) = 2i \ln 2 \frac{e^2 T}{\pi \hbar \omega}$$

and it depends on temperature.

The behavior of such type can be observed on experiments involving the plasmon modes. The dispersion law of such modes for 2D systems is gapless,

$$\omega = v_0 \sqrt{\kappa k}, \quad \kappa = \frac{2e^2 T \ln 2}{\hbar^2 v_0^2 \varepsilon_\infty},$$

where ε_{∞} is the lattice dielectric constant.

So far we considered the 2D graphene sheet. The results obtained can be immediately applied to the 3D graphite if one neglect the interaction between the layers. Then the integration with respect to the p_z component of the quasi-momentum in the Brillouin zone gives just the additional factor $1/c_z$ in comparison with the conductivity of graphene, where c_z is the distance between the layers in the z-direction. For instance, Eqs. (9) and (10) acquire the factor $1/c_z$. In the low-frequency limit $\omega \ll 1/\tau$, conductivity can be estimated as

$$\sigma^{(3)}(\omega, k \to 0) = 2 \ln 2 \frac{e^2 T \tau}{\pi \hbar c_z}.$$

The number of phonons in the 2D graphene at low temperatures ($T \ll T_D, T_D$ is the Debye temperature) is proportional to T^2 . Since the Fermi surface is assumed to be small ($\varepsilon_F < T < T_D$), all scattering angles are essential in this region of temperatures. For the electron collision rate, which is determined by the electron-phonon interaction, one can write $\tau^{-1} = \alpha T^2/T_D$ with the constant α of the order of unity. Thus the in-layer resistivity turns out to be linear in temperature:

$$\rho = \frac{\pi \hbar \alpha c_z T}{2e^2 T_D \ln 2} = 320 \frac{\alpha T}{T_D} \,\mu\Omega \,\text{cm}. \tag{17}$$

According to Ref. [8], $\rho=60~\mu\Omega\,\mathrm{cm}$ at $T=300~\mathrm{K}$ in agreement with the above estimate $(T_D\simeq 2000K$ for graphite, $\alpha\sim 1)$. The equation (17) answers the question discussed in Refs. [8, 9] on the pressure dependence of the graphite resistivity. We see that the resistivity decreases under the pressure because the inter-layer distance c_z decreases and the Debye temperature T_D grows.

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